Transport in disordered interacting systems: Numerical results for one-dimensional spinless electrons

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Abstract

The combined influence of disorder and interactions on the transport properties of electrons in one dimension is investigated. The numerical simulations are carried out by means of the Hartree-Fock-based diagonalization (HFD), a very efficient method to determine the low-energy properties of a disordered many-particle system. We find that the conductance of a strongly localized system can become considerably enhanced by the interactions. The enhancement for long-range interactions is significantly larger than for short-range interactions. In contrast, the conductance of weakly localized systems becomes suppressed by the interactions.

The transport properties of disordered electrons have been a subject of continuous interest within the last 4 decades. In 1958 Anderson pointed out [1] that the electronic (single-particle) wave function may become localized in space for sufficiently strong disorder. For one-dimensional systems it was later proved rigorously that all states are exponentially localized for arbitrary finite disorder [2–4]. Further investigations of *non-interacting* disordered electrons led to the development of the scaling theory of localization [5,6]. It predicts that in the absence of a magnetic field or spin-orbit coupling all states are localized not only in one but also in two dimensions. Thus a metallic state does not exist in these dimensions. In contrast, in three dimensions states are extended for weak disorder while they are localized for sufficiently strong disorder. This gives rise to a disorder-driven metal-insulator transition (MIT) at a certain value of disorder strength.

Later also the influence of electron-electron interactions on the transport properties of disordered electrons was investigated intensively by means of many-body perturbation theory [7], scaling theory [8], and the renormalization group (for reviews see. e.g. [9–11]). This led to a qualitative analysis of the MIT and the identification of the different universality classes. One of the main results is that the lower critical dimension of the MIT is $d_c^- = 2$ as it is for

non-interacting electrons [11]. Therefore it came as a surprise when measurements [12] on Si-MOSFETs revealed indications of a MIT in 2D. Since these experiments are carried out at low electron density where the Coulomb interaction is particularly strong compared to the Fermi energy, interaction effects are the most likely reason for this phenomenon. A complete understanding has, however, not yet been obtained. There have been attempts to explain the experiments based on the perturbative renormalization group [13], non-perturbative effects [14], or the transition being a superconductor-insulator transition rather than a MIT [15].

In view of all this it seems to be important to investigate the problem of interacting disordered electrons not only in the perturbative regime (of weak disorder and interactions) but also for strong disorder or/and interactions. Recently, we investigated [16] the transport properties of two-dimensional disordered interacting electrons. We found that weak interactions enhance the conductance in the strongly localized regime while they reduce the conductance in the case of weaker disorder. In contrast, sufficiently strong interactions always reduce the conductance.

In this paper we extend this study to the case of one dimension. We report numerical results for the conductance of a simple model system of interacting disordered electrons, viz. spinless fermions in a random potential interacting via Coulomb or short-range interactions. Our results cover the entire parameter range from weak disorder and interactions to strong disorder and interactions. The model, a one-dimensional version of the quantum Coulomb glass model [17–20], is defined on a ring (using periodic boundary conditions) of L sites occupied by $N = KL$ electrons ($0 < K < 1$). To ensure charge neutrality each lattice site carries a compensating positive charge of Ke. The Hamiltonian is given by

$$H = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) + \sum_i \varphi_i n_i + \frac{1}{2} \sum_{i \neq j} (n_i - K)(n_j - K) U_{ij} \qquad (1)$$

where $c_i^\dagger$ and c_i are the electron creation and annihilation operators at site i, respectively, and $\langle ij \rangle$ denotes all pairs of nearest neighbor sites. t gives the strength of the hopping term and n_i is the occupation number of site i. For a correct description of the insulating phase the Coulomb interaction between the electrons is kept long-ranged, $U_{ij} = U/r_{ij}$, since screening breaks down in the insulator (r_{ij} is measured in units of the lattice constant). For comparison we also investigate the case of nearest neighbor interaction of strength U. The random potential values φ_i are chosen independently from a box distribution of width $2W$ and zero mean. (In the following we always set $W = 1$.) Two important limiting cases of the quantum Coulomb glass are the Anderson model of localization (for $U_{ij} = 0$) and the classical Coulomb glass (for $t = 0$).

The simulation of disordered quantum many-particle systems is numerically very costly since the size of the Hilbert space grows exponentially with system size and since many disorder configurations have to be considered to obtain typical values or distribution functions of observables. We have recently developed the Hartree-Fock based diagonalization (HFD) method [16] for the simulation of disordered quantum many-particle systems. This method which is based on the idea of the configuration interaction approach [21] adapted to disordered lattice models is very efficient in calculating low-energy properties in any spatial dimension and for short-range as well as long-range interactions. It consists of 3 steps: (i) solve the Hartree-Fock (HF) approximation of the Hamiltonian, (ii) use a Monte-Carlo algorithm to find the low-energy many-particle HF states, (iii) diagonalize the Hamiltonian in the basis formed by these states. The efficiency of the HFD method is due to the fact that the HF basis states are comparatively close in character to the exact eigenstates in the entire parameter space [22]. Thus it is sufficient to keep only a small fraction of the Hilbert space in order to obtain low-energy quantities with an accuracy comparable to that of exact diagonalization. For the present study we have simulated rings with 24 sites and 12 electrons. For this size we found it sufficient to keep 500 to 1000 (out of 2704156) basis states.

The conductance is calculated from the Kubo-Greenwood formula [23] which connects the conductance with the current-current correlation function in the ground state. Using the spectral representation of the correlation function the real (dissipative) part of the conductance (in units of the quantum conductance e^2/h) is obtained as

$$\Re \, G^{xx}(\omega) = \frac{2\pi^2}{L\omega} \sum_{\nu} |\langle 0|j^x|\nu\rangle|^2 \delta(\omega + E_0 - E_\nu) \tag{2}$$

where j^x is the x component of the current operator and ν denotes the eigenstates of the Hamiltonian. The finite life time τ of the eigenstates in a real d.c. transport experiment (where the system is not isolated but connected to contacts and leads) results in an inhomogeneous broadening $\gamma = 1/\tau$ of the δ functions in the Kubo-Greenwood formula [24]. Here we have chosen $\gamma = 0.05$ which is of the order of the single-particle level spacing.

We now present results on the dependence of the conductance on the interaction strength. In Figs. 1 and 2 we show the conductance as a function of frequency for two sets of parameters. The data represent logarithmic averages over 400 disorder configurations. In Fig. 1 the kinetic energy is very small ($t = 0.03$). Thus the system is in the highly localized regime, as we have also estimated from the single-particle participation number which is smaller than 2. Here not too strong Coulomb interactions ($U = 0.5, 1.0$) lead to an *increase* of the conductance at low frequencies. If the interaction becomes stronger ($U = 2$) the conductance finally decreases again. The behavior is qualitatively
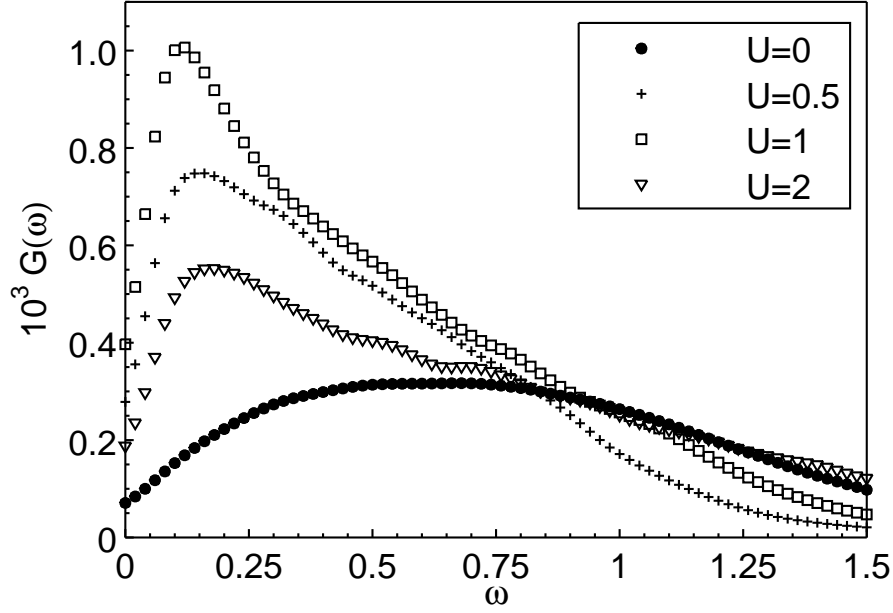
Fig. 1. Conductance G as a function of frequency ω, $W = 1$, $t = 0.03$, $\gamma = 0.05$. The truncation of the Hilbert space to 500 basis states restricts the validity of these data to frequencies $\omega < 0.75$.
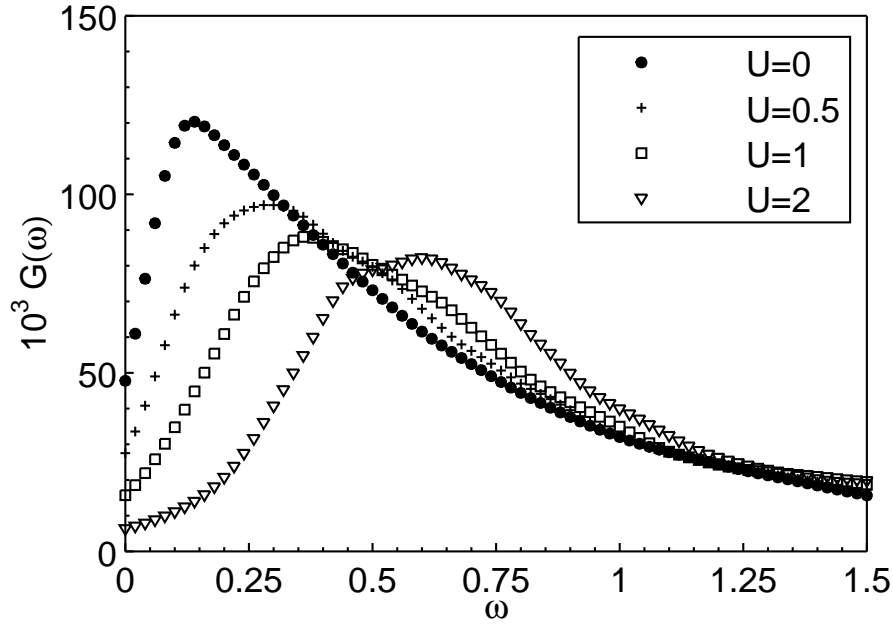

Fig. 2. Same as Fig. 1 but for $t = 0.5$.

different at higher kinetic energy ($t = 0.5$) as shown in Fig. 2. Here the localization is much weaker (the single-particle participation number is of the order of 10). Already a weak interaction ($U = 0.5$) leads to a reduction of the low-frequency conductance compared to non-interacting electrons. If the
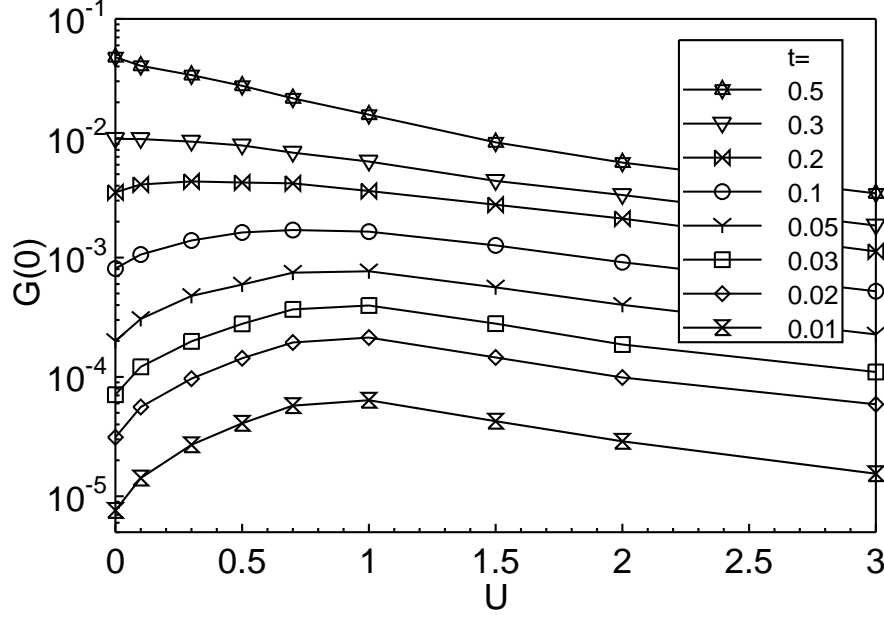
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Fig. 3. d.c. conductance $G(0)$ as a function of interaction strength U for different kinetic energies t.

interaction becomes stronger ($U = 2$) the conductance decreases further.

We have carried out analogous calculations for kinetic energies $t = 0.01, ..., 0.5$ and interaction strengths $U = 0, ..., 3$. The resulting d.c. conductances are presented in Fig. 3 which is the main result of this paper. It shows that the influence of weak repulsive electron-electron interactions on the d.c. conductance is opposite in the cases of weak and strong disorder. Sufficiently strong interactions always reduce the conductance. This is not surprising since strong interactions will reduce charge fluctuations and in the limit of infinite interaction strength the system approaches a Wigner crystal. In contrast, the effect of weak (compared to the random potential) interactions depends on the value t of the kinetic energy. The conductance of strongly localized samples ($t = 0.01, ..., 0.05$) becomes considerably enhanced by a weak Coulomb interaction. In this regime the dominant effect is the suppression of the localizing interference effects by electron-electron scattering events. With increasing kinetic energy the relative enhancement decreases as does the interaction range where the enhancement occurs. The conductance of samples with high kinetic energies ($t \geq 0.3$) is reduced even by weak interactions. Here the dominant effect is the suppression of charge fluctuations by the interactions. Overall, only the behavior at high kinetic energies (i.e. weak disorder) is in agreement with analytical results based on the perturbative renormalization group [25] while the behavior for low kinetic energy (strong disorder) is qualitatively different.

For comparison we have also investigated nearest-neighbor interactions instead of long-range Coulomb interactions. In Fig. 4 we compare the d.c. con-
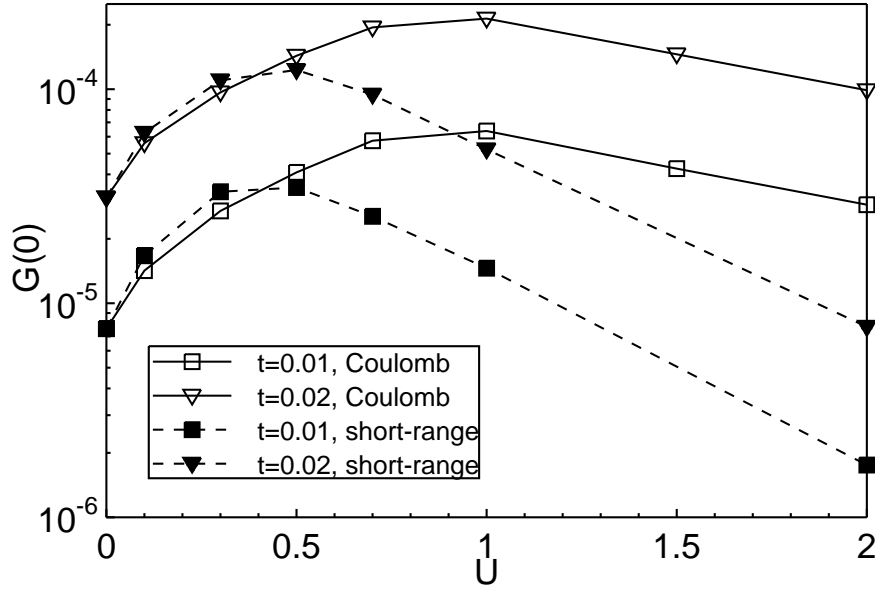
Fig. 4. d.c. conductance $G(0)$ as a function of interaction strength U for short- and long-range interactions. The data represent logarithmic averages over 400 disorder configurations.

ductances of systems with short- and long-range interactions in the localized regime. The data show that the interaction induced enhancement of the conductance is overall weaker in the case of short range interactions. In particular, the maximum enhancement as a function of interaction strength is significantly smaller (by a factor of about two) than in the Coulomb case. Moreover, the maximum occurs for weaker interaction strength.

In the last part of this paper we want to relate our findings to the two-dimensional case [16] and to results in the literature. The qualitative dependence of the d.c. conductance on kinetic energy and interaction is identical in one and two spatial dimensions. The interaction-induced enhancement in the localized regime is, however, significantly larger in the one-dimensional systems investigated. Up to now it is not clear whether this is a true dimensionality effect or a result of the different linear system sizes studied. In order to resolve this question a systematic investigation of the system size dependence is in progress [26]. The resulting scaling behavior of the conductance with system size will also allow us to check for the existence of an interaction-induced MIT. Note, however, that the recently observed MIT in 2D MOSFETs [12] is not likely to be explained by the enhancement of the conductance we found since the importance of the spin degrees of freedom for this transition is well established experimentally [27]. We emphasize, however, that our numerical method is very easy to generalize to electrons with spin. The fact that we find the strongest enhancement of the conductance for very low kinetic energy also

suggests that the mechanism is different from that giving rise to an increased two-particle localization length in the problem of just two interacting particles [28] (where the strongest delocalization is observed for weak disorder). Let us finally mention that the conclusions drawn in this paper are in qualitative agreement with those of a recent DMRG study [29] of the phase sensitivity of the ground state energy for a disordered one-dimensional model of spinless fermions with nearest-neighbor interactions which showed that for small disorder repulsive interactions reduce the phase sensitivity while for large disorder the phase sensitivity shows pronounced enhancements at certain values of the interaction.

To summarize, we have used the Hartree-Fock based diagonalization (HFD) method to investigate the conductance and localization properties of disordered interacting spinless electrons in one dimension. We have found that a weak Coulomb interaction can enhance the conductivity of strongly localized samples by almost one order of magnitude, while it reduces the conductance of weakly disordered samples. If the interaction becomes stronger it eventually reduces the conductance also in the localized regime. The interaction induced enhancement is larger for long-range interactions than for short-range interactions.

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